Day :
Friday
Date:
6/25/2004

Time:
16:00:36

PALM INTRANET

Inventor Information for 10/627483

Inventor Name	City	State/Country
WU, YE	HELOTES	TEXAS
KOCHAT, HARRY	SAN ANTONIO	TEXAS

Appln Info | Contents | Petition Info | Atty/Agent Info | Continuity Data | Foreig

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10/627,483 Thomas McKenzie

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FILE 'HOME' ENTERED AT 16:24:51 ON 25 JUN 2004

=> file casreacts
'CASREACTS' IS NOT A VALID FILE NAME
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Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

```
=> file casreact
FILE 'CASREACT' ENTERED AT 16:25:12 ON 25 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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FILE CONTENT:1840 - 20 Jun 2004 VOL 140 ISS 25

************************************************************
*                                                          *
*     CASREACT now has more than  8 million reactions      *
*                                                          *
************************************************************

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file
and provided by InfoChem and some records are produced using some INPI
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This file contains CAS Registry Numbers for easy and accurate substance
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Crossover limits have been increased.  See HELP RNCROSSOVER for details.

Structure search limits have been raised.  See HELP SLIMIT for the new,
higher limits.

=>
Uploading C:\Program Files\Stnexp\Queries\10627483.str
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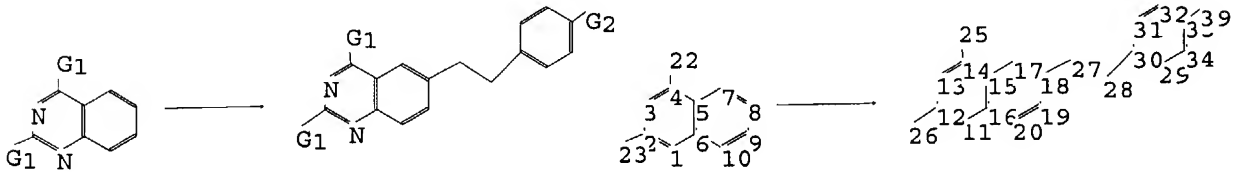


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chain nodes :
22  23  25  26  27  28  35  36  39
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  29  30  31
32  33  34
chain bonds :
2-23  4-22  12-26  14-25  18-27  27-28  28-30  33-39  35-36
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  11-12  11-16  12-13  13-14
 14-15  15-16  15-17  16-20  17-18  18-19  19-20  29-30  29-34  30-31  31-32  32-33
 33-34
exact/norm bonds :
```

```
2-23  4-22  12-26  14-25  33-39  35-36
exact bonds :
18-27  27-28  28-30
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  11-12  11-16  12-13  13-14
 14-15  15-16  15-17  16-20  17-18  18-19  19-20  29-30  29-34  30-31  31-32  32-33
 33-34


G1:C,O,N

G2:OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,[*1]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  22:CLASS  23:CLASS  25:CLASS  26:CLASS  27:CLASS  28:CLASS  29:Atom
30:Atom  31:Atom  32:Atom  33:Atom  34:Atom  35:CLASS  36:CLASS  39:CLASS
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1



L1      STRUCTURE UPLOADED

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SAMPLE SEARCH INITIATED 16:29:08 FILE 'CASREACT'
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100.0% DONE      0 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:         0 TO        0
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1 (     0 REACTIONS)

=> s l1 full
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SCREENING COMPLETE -     36 REACTIONS TO VERIFY FROM      5 DOCUMENTS

100.0% DONE     36 VERIFIED      23 HIT RXNS                      3 DOCS
SEARCH TIME: 00.00.01

L3            3 SEA SSS FUL L1 (    23 REACTIONS)

=> d 1-3

L3   ANSWER 1 OF 3  CASREACT  COPYRIGHT 2004 ACS on STN

RX(1) OF 40 - REACTION DIAGRAM NOT AVAILABLE

L3   ANSWER 2 OF 3  CASREACT  COPYRIGHT 2004 ACS on STN
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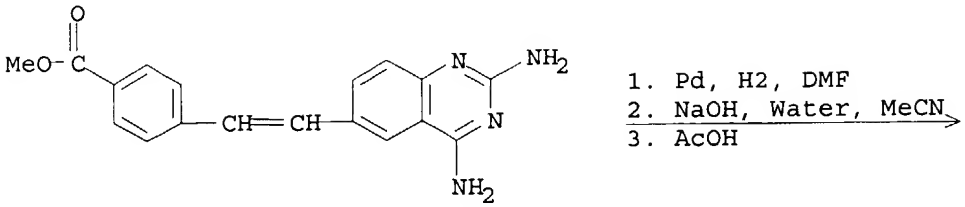
RX(5) OF 28



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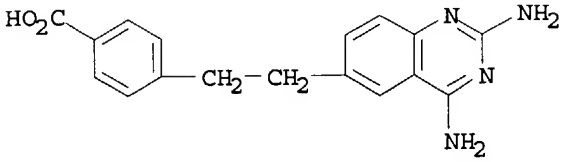
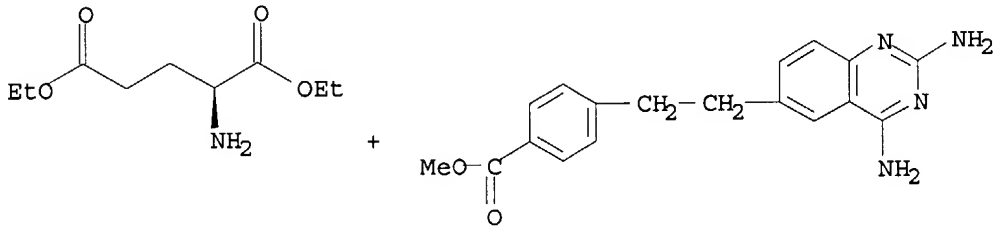


REF: Medicinal Chemistry Research, 9(3), 176-185; 1999

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2004 ACS on STN

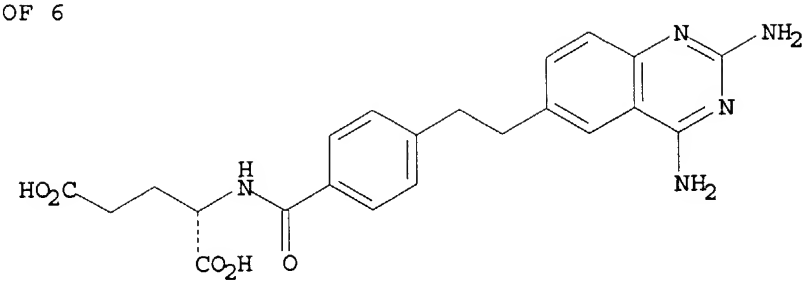
RX(1) OF 6



HCl
(step 2)

(step 1)

RX(1) OF 6



17%

REF: Synlett, (10), 577-8; 1990

=> d 1 cbib pi hitrxn
'HITRXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"

FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

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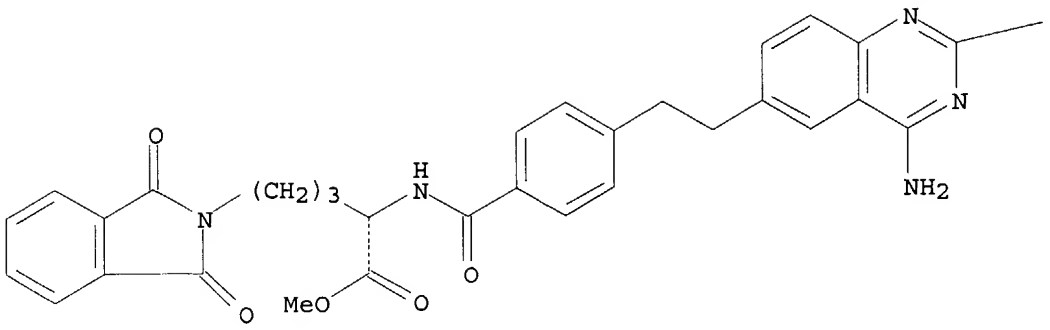
ENTER DISPLAY FORMAT (FCRDREF):cbib pi rx rxs

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2004 ACS on STN
136:386360 Synthesis and In Vitro Antitumor Activity of New Deaza Analogues of the Nonpolyglutamatable Antifolate Nα-(4-Amino-4-deoxypteroyl)-Nδ-hemiphthaloyl-L-ornithine (PT523). Vaidya, Chitra M.; Wright, Joel E.; Rosowsky, Andre (Dana-Farber Cancer Institute and the Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA). Journal of Medicinal Chemistry, 45(8), 1690-1696 (English) 2002. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.

RX(1) OF 40 ...**A** ===> **B**

PAGE 1-A



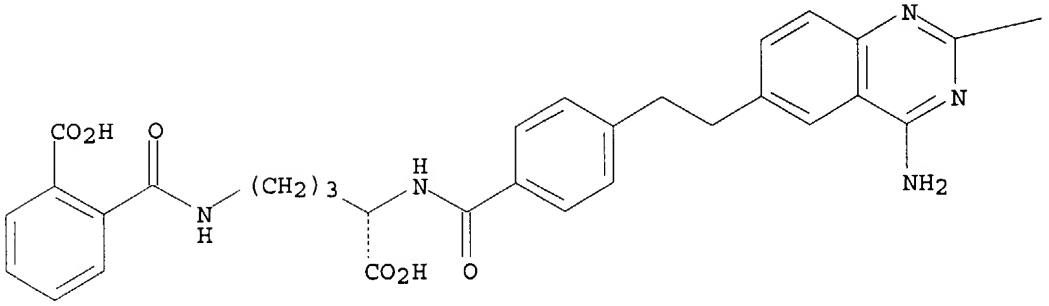
PAGE 1-B

—NH_2

A

(1) →

PAGE 1-A



PAGE 1-B

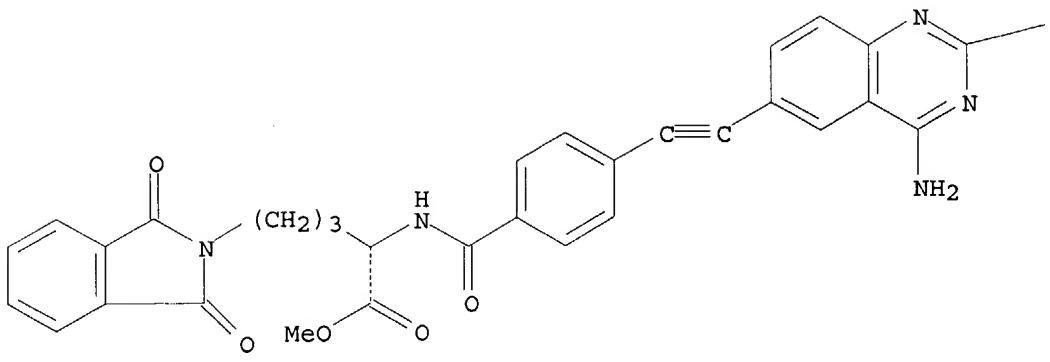
—NH_2

B
YIELD 40%

RX(1) RCT A **425623-45-6**
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) OF 40 ...**X** ===> **A**...

PAGE 1-A



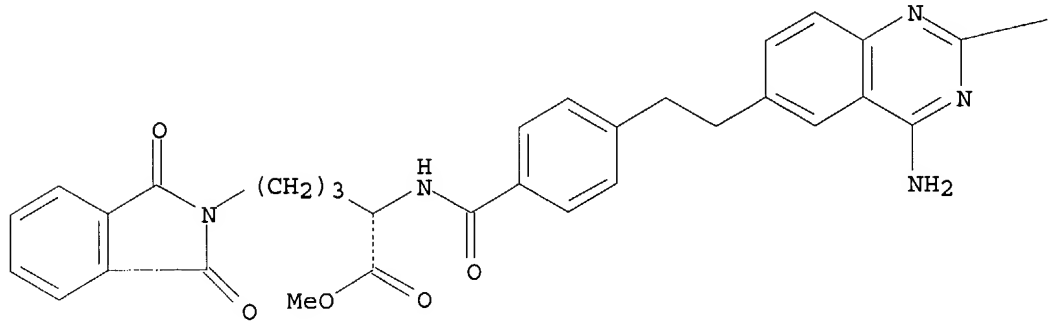
PAGE 1-B

—NH_2

X

(7) →

PAGE 1-A



PAGE 1-B

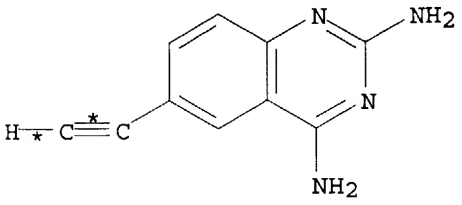
—NH_2

A
YIELD 62%

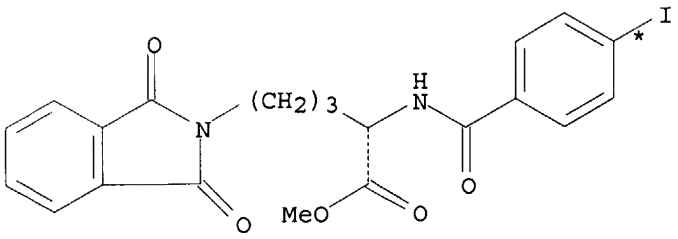
RX(7) RCT X **425623-44-5**

RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(15) OF 40 COMPOSED OF RX(6), RX(7)
RX(15) **O** + **J** ===> **A**



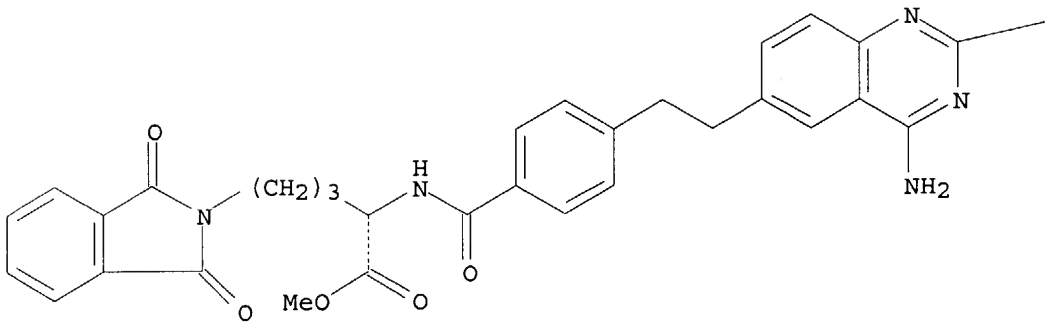
O



J

2
STEPS

PAGE 1-A



PAGE 1-B

—NH2

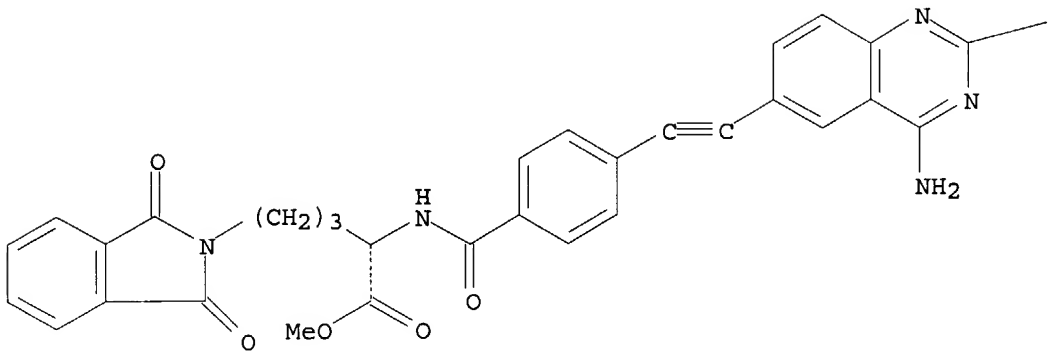
A
YIELD 62%

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(16) OF 40 COMPOSED OF RX(7), RX(1)
RX(16) **X** ===> **B**

PAGE 1-A



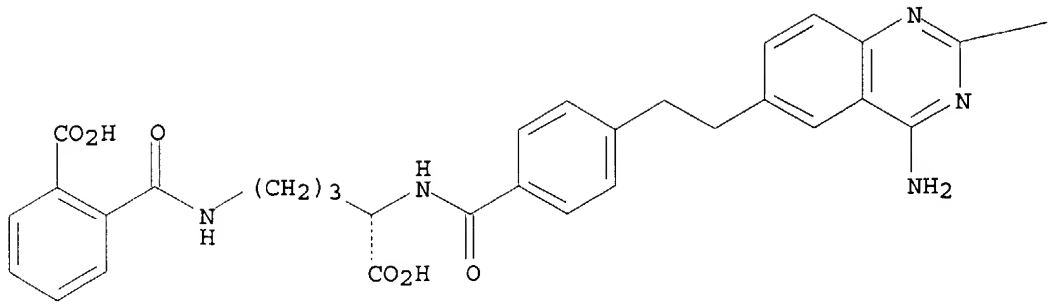
PAGE 1-B

—NH2

X

2
STEPS

PAGE 1-A



PAGE 1-B

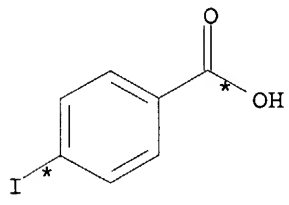
—NH_2

B
YIELD 40%

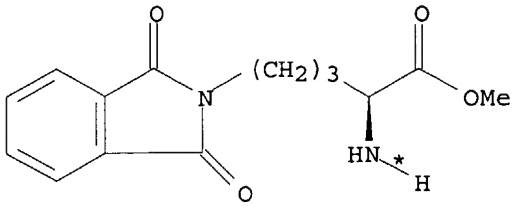
RX(7) RCT X **425623-44-5**
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(22) OF 40 COMPOSED OF RX(3), RX(6), RX(7)
RX(22) H + I + **O** ===> **A**



H



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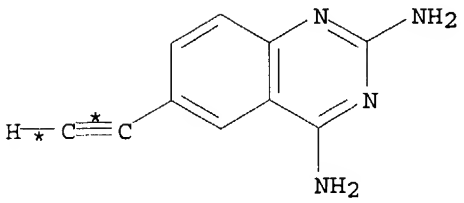
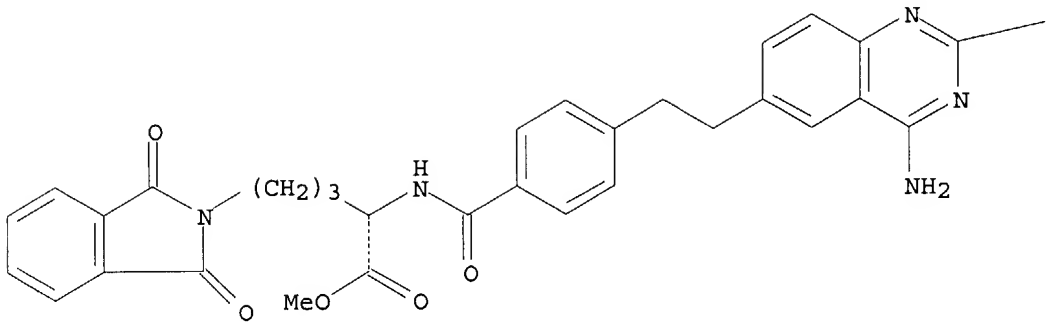


3
STEPS

O

PAGE 1-A



PAGE 1-B

—NH_2

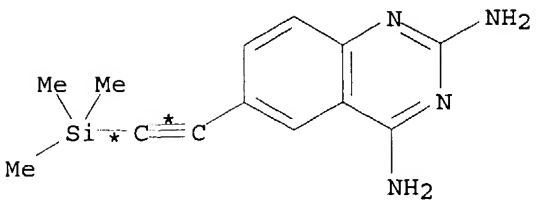
A
YIELD 62%

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(23) OF 40 COMPOSED OF RX(4), RX(6), RX(7)
RX(23) **N + J ===> A**



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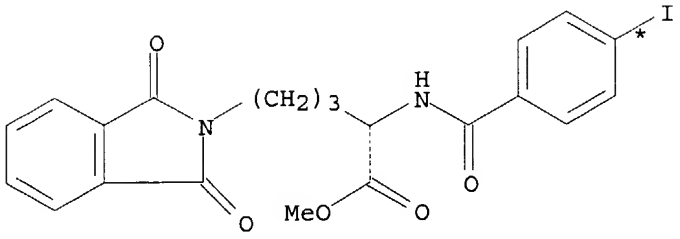
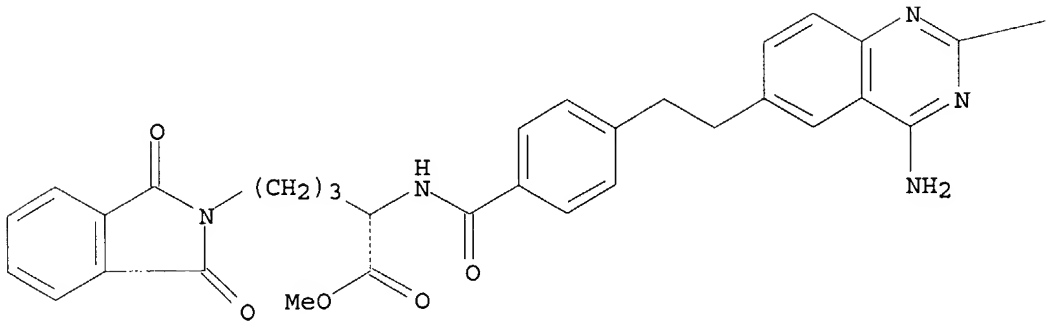


J

3
STEPS

PAGE 1-A



PAGE 1-B

—NH_2

A
YIELD 62%

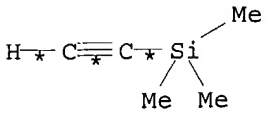
RX(4) RCT N **425623-43-4**
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5

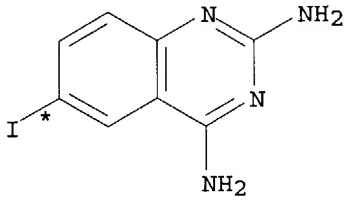
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(25) OF 40 COMPOSED OF RX(5), RX(4), RX(6), RX(7)
RX(25) R + **S** + J ===> **A**



R



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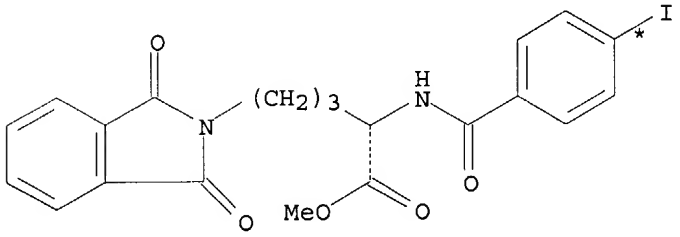
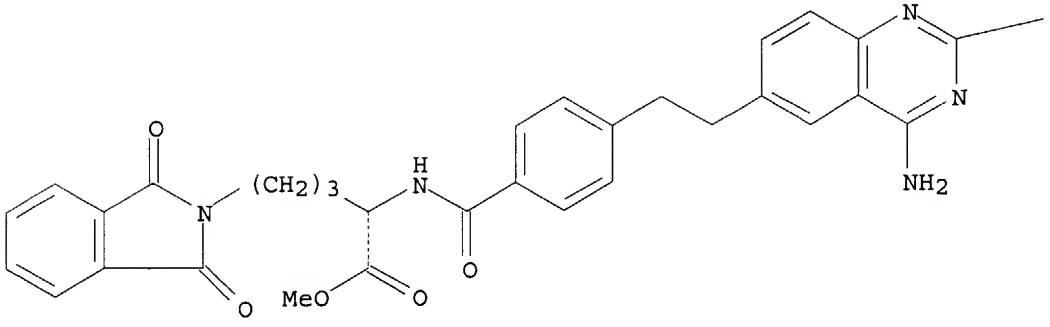


J

4
STEPS

PAGE 1-A



—NH_2

A
YIELD 62%

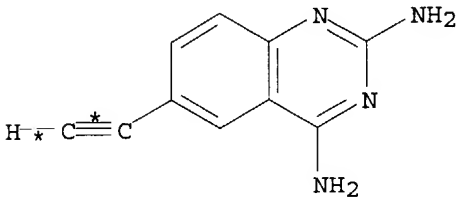
RX(5) RCT R 1066-54-2, S **132131-20-5**
RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2
Tri-o-tolylphosphine
SOL 68-12-2 DMF

RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

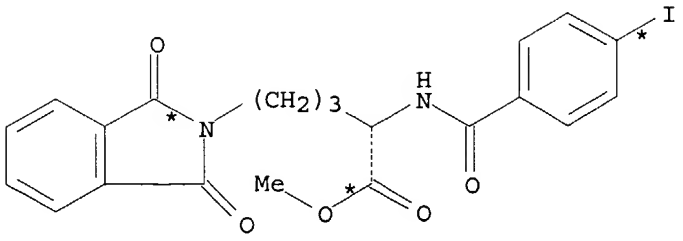
RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(27) OF 40 COMPOSED OF RX(6), RX(7), RX(1)
RX(27) **O** + J ===> **B**



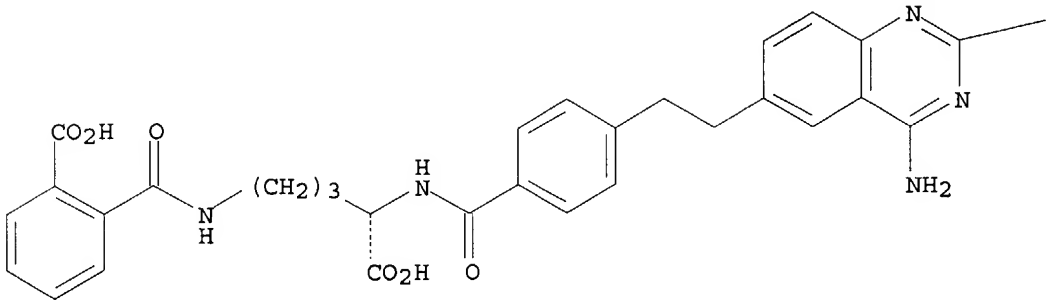
O



3
STEPS

J

PAGE 1-A



PAGE 1-B

—NH_2

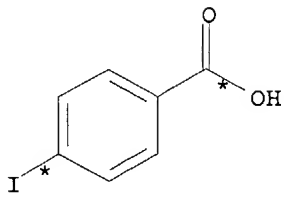
B
YIELD 40%

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

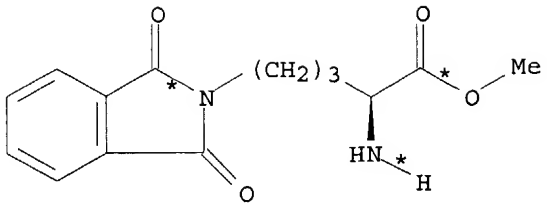
RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

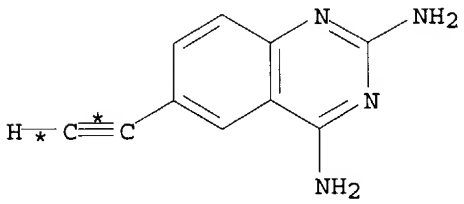
RX(28) OF 40 COMPOSED OF RX(3), RX(6), RX(7), RX(1)
RX(28) H + I + **O** ===> **B**



H



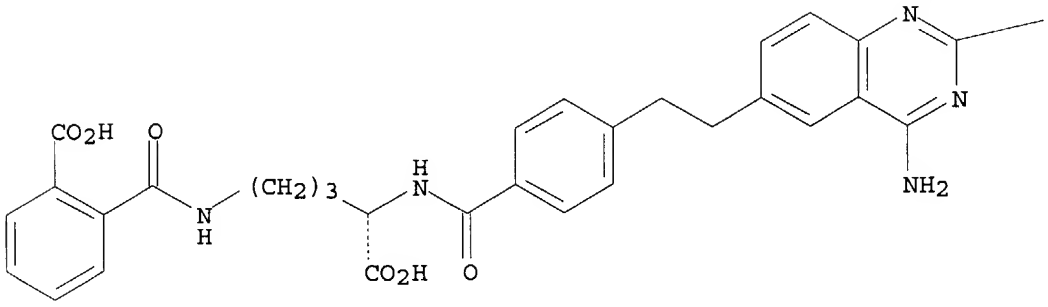
I



O

4
STEPS

PAGE 1-A



PAGE 1-B

—NH_2

B
YIELD 40%

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

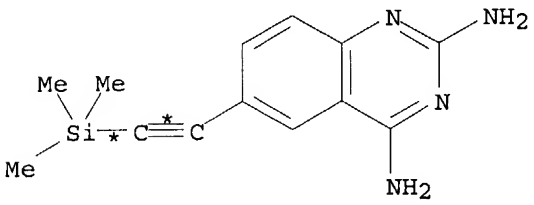
RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4

SOL 68-12-2 DMF

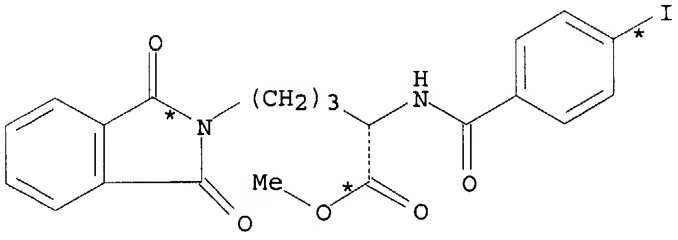
RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(29) OF 40 COMPOSED OF RX(4), RX(6), RX(7), RX(1)
RX(29) **N** + J ===> **B**



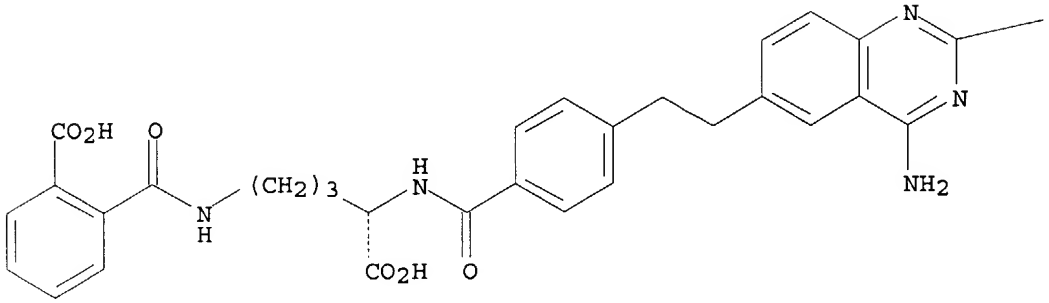
N



J

4
STEPS

PAGE 1-A



—NH_2

B
YIELD 40%

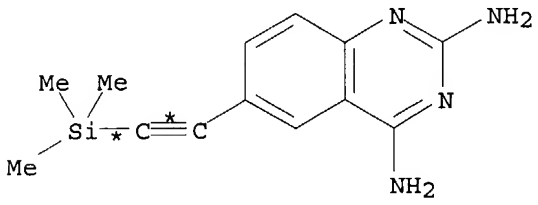
RX(4) RCT N **425623-43-4**
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

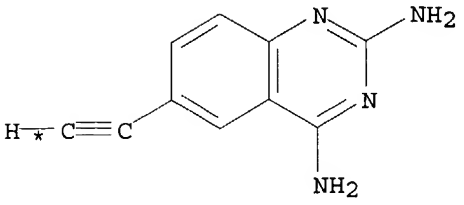
RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(35) OF 40 COMPOSED OF REACTION SEQUENCE RX(4), RX(6), RX(7)
AND REACTION SEQUENCE RX(3), RX(6), RX(7)
...N ===> O...
...H + I + **O** ===> **A**



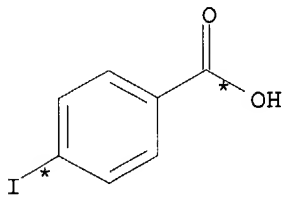
3
STEPS

N

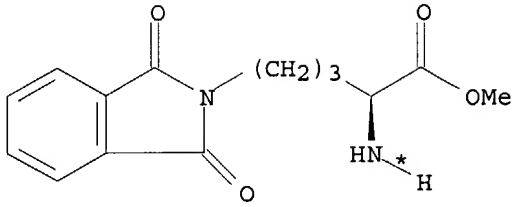


O

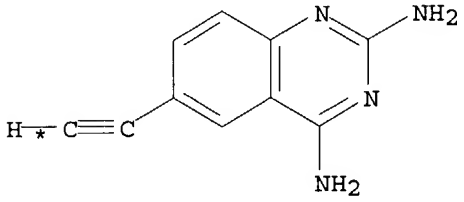
START NEXT REACTION SEQUENCE



H



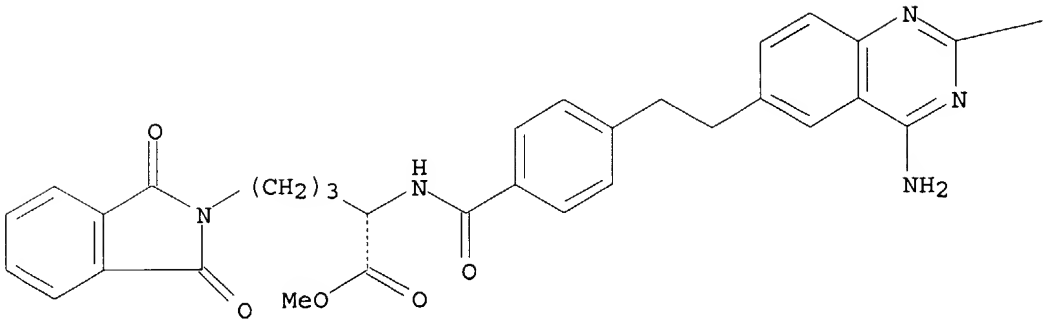
I



O

3
STEPS

PAGE 1-A



A
YIELD 62%

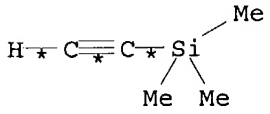
RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

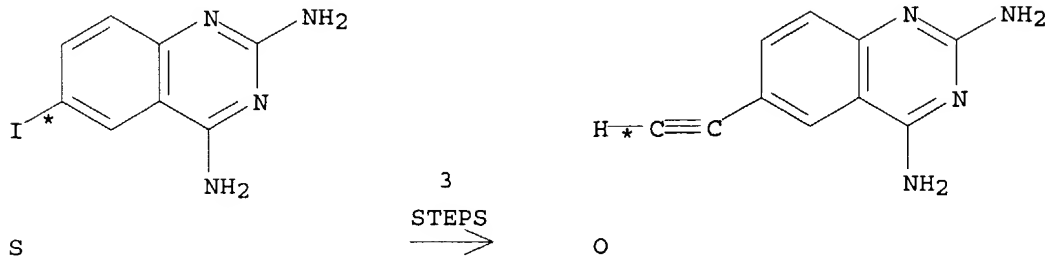
RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(36) OF 40 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(6), RX(7)
AND REACTION SEQUENCE RX(3), RX(6), RX(7)
...R + S ===> O...
...H + I + **O** ===> **A**

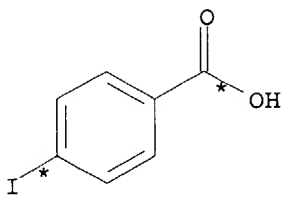


R

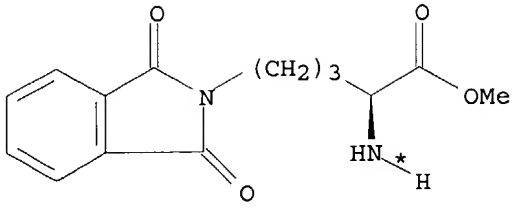


S O

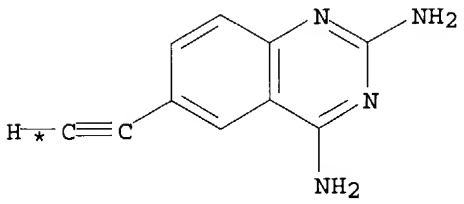
START NEXT REACTION SEQUENCE



H



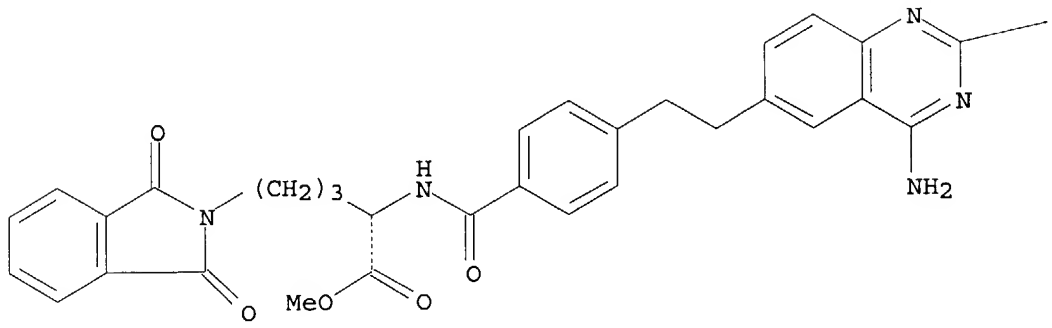
I



O

3
STEPS

PAGE 1-A



PAGE 1-B

—NH_2

A
YIELD 62%

RX(5) RCT R 1066-54-2, S 132131-20-5
RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2
Tri-o-tolylphosphine
SOL 68-12-2 DMF

RX(4) RCT N 425623-43-4

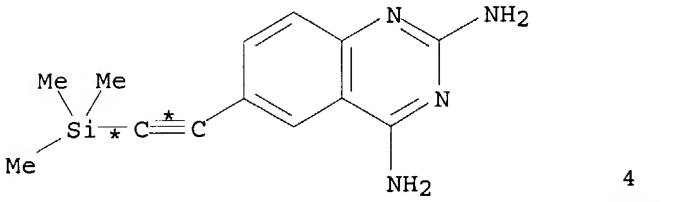
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

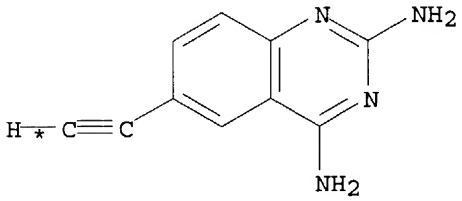
RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(37) OF 40 COMPOSED OF REACTION SEQUENCE RX(4), RX(6), RX(7), RX(1)
AND REACTION SEQUENCE RX(3), RX(6), RX(7), RX(1)
...N ===> O...
...H + I + **O** ===> **B**

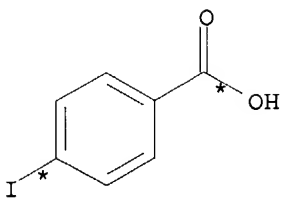


N

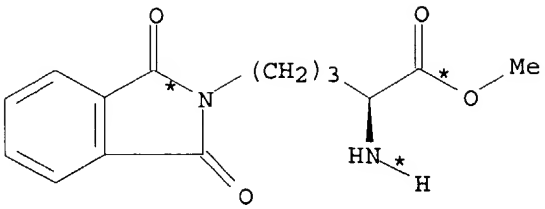


O

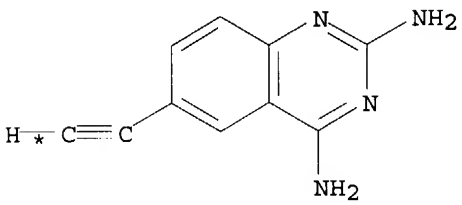
START NEXT REACTION SEQUENCE



H



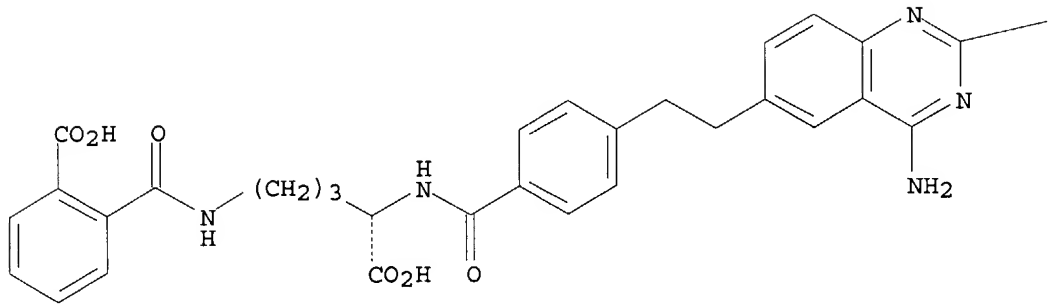
I



O

4
STEPS

PAGE 1-A



PAGE 1-B

—NH2

B
YIELD 40%

RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2

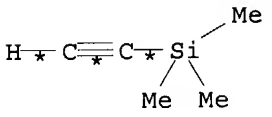
SOL 68-12-2 DMF

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

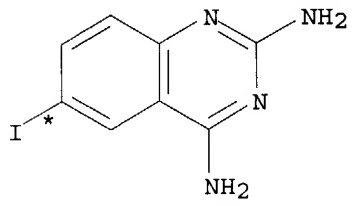
RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

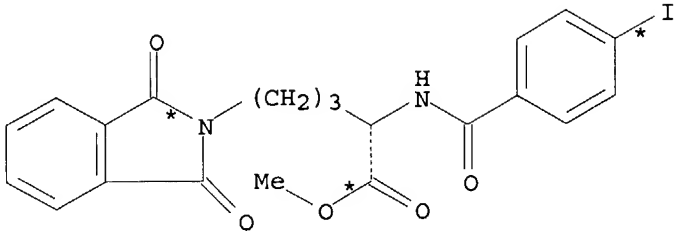
RX(38) OF 40 COMPOSED OF RX(5), RX(4), RX(6), RX(7), RX(1)
RX(38) R + **S** + J ===> **B**



R



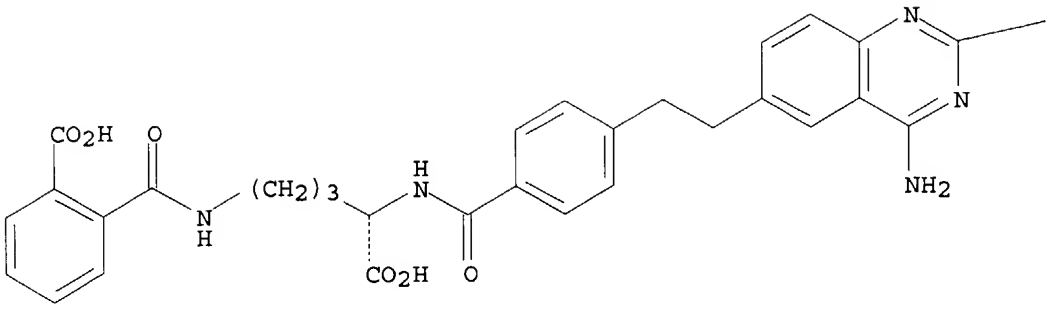
S



J

5
STEPS

PAGE 1-A



PAGE 1-B

—NH_2

B
YIELD 40%

RX(5) RCT R 1066-54-2, S **132131-20-5**
RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2 Tri-o-tolylphosphine
SOL 68-12-2 DMF

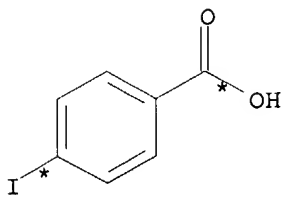
RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

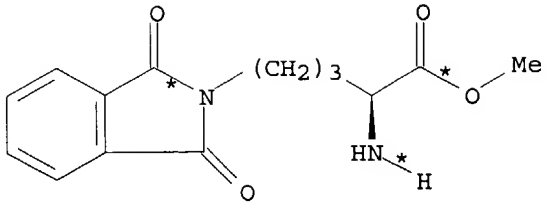
RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(39) OF 40 COMPOSED OF REACTION SEQUENCE RX(3), RX(6), RX(7), RX(1)
AND REACTION SEQUENCE RX(5), RX(4), RX(6), RX(7), RX(1)
...H + I ===> J...
...R + **S** + J ===> **B**

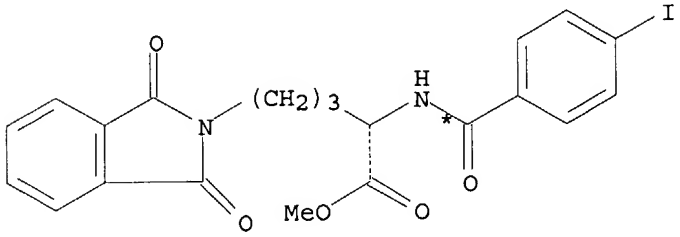


H



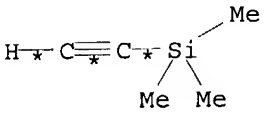
I

5
STEPS



J

START NEXT REACTION SEQUENCE



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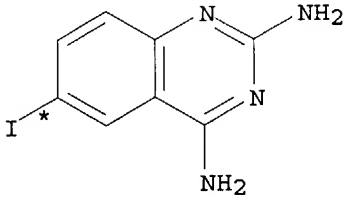

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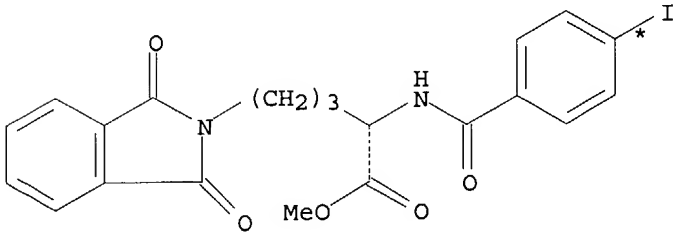
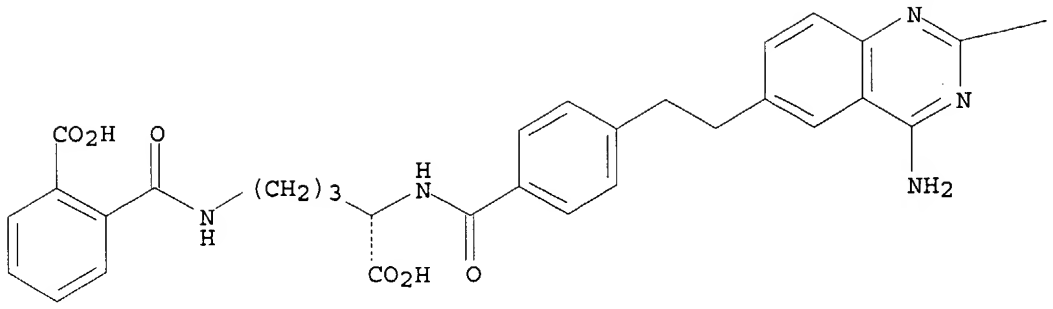


J

5
STEPS

PAGE 1-A



PAGE 1-B

—NH_2

B
YIELD 40%

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(5) RCT R 1066-54-2, S **132131-20-5**
RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2
Tri-o-tolylphosphine
SOL 68-12-2 DMF

RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(1) OF 40 ...**A** ===> **B**

RX(1) RCT A **425623-45-6**
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) OF 40 ...**X** ===> **A**...

RX(7) RCT X **425623-44-5**
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(15) OF 40 COMPOSED OF RX(6), RX(7)
RX(15) **O** + J ===> **A**

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(16) OF 40 COMPOSED OF RX(7), RX(1)
RX(16) **X** ===> **B**

RX(7) RCT X **425623-44-5**
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(22) OF 40 COMPOSED OF RX(3), RX(6), RX(7)
RX(22) H + I + **O** ===> **A**

RX(3) RCT H 619-58-9, I 66024-35-9

RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(23) OF 40 COMPOSED OF RX(4), RX(6), RX(7)
RX(23) **N** + J ===> **A**

RX(4) RCT N **425623-43-4**
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(25) OF 40 COMPOSED OF RX(5), RX(4), RX(6), RX(7)
RX(25) R + **S** + J ===> **A**

RX(5) RCT R 1066-54-2, S **132131-20-5**
RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2
Tri-o-tolylphosphine
SOL 68-12-2 DMF

RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(27) OF 40 COMPOSED OF RX(6), RX(7), RX(1)
RX(27) **O** + **J** ===> **B**

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(28) OF 40 COMPOSED OF RX(3), RX(6), RX(7), RX(1)
RX(28) H + I + **O** ===> **B**

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(29) OF 40 COMPOSED OF RX(4), RX(6), RX(7), RX(1)
RX(29) **N** + **J** ===> **B**

RX(4) RCT N **425623-43-4**
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(35) OF 40 COMPOSED OF REACTION SEQUENCE RX(4), RX(6), RX(7)
AND REACTION SEQUENCE RX(3), RX(6), RX(7)
...N ===> O...
...H + I + **O** ===> **A**

RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(6) RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(36) OF 40 COMPOSED OF REACTION SEQUENCE RX(5), RX(4), RX(6), RX(7)
AND REACTION SEQUENCE RX(3), RX(6), RX(7)
...R + S ===> O...
...H + I + **O** ===> **A**

RX(5) RCT R 1066-54-2, S 132131-20-5

RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2 Tri-o-tolylphosphine
SOL 68-12-2 DMF

RX(4)
RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(3)
RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(6)
RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7)
RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A **425623-45-6**
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(37) OF 40 COMPOSED OF REACTION SEQUENCE RX(4), RX(6), RX(7), RX(1) AND REACTION SEQUENCE RX(3), RX(6), RX(7), RX(1)

...N ===> O...
...H + I + **O** ===> **B**

RX(4)
RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(3)
RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(6)
RCT O **425623-42-3**, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7)
RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1)
RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**

SOL 67-56-1 MeOH, 7732-18-5 Water

RX(38) OF 40 COMPOSED OF RX(5), RX(4), RX(6), RX(7), RX(1)
RX(38) R + **S** + J ===> **B**

RX(5) RCT R 1066-54-2, S **132131-20-5**
RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2
Tri-o-tolylphosphine
SOL 68-12-2 DMF

RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

RX(6) RCT O 425623-42-3, J 425623-41-2
RGT L 121-44-8 Et3N
PRO X 425623-44-5
CAT 14221-01-3 Pd(PPh3)4
SOL 68-12-2 DMF

RX(7) RCT X 425623-44-5
RGT Z 1333-74-0 H2
PRO A 425623-45-6
CAT 7440-05-3 Pd
SOL 75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1) RCT A 425623-45-6
RGT C 17194-00-2 Ba(OH)2
PRO B **425623-39-8**
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(39) OF 40 COMPOSED OF REACTION SEQUENCE RX(3), RX(6), RX(7), RX(1)
AND REACTION SEQUENCE RX(5), RX(4), RX(6), RX(7), RX(1)
...H + I ===> J...
...R + **S** + J ===> **B**

RX(3) RCT H 619-58-9, I 66024-35-9
RGT K 543-27-1 ClCO2Bu-i, L 121-44-8 Et3N
PRO J 425623-41-2
SOL 68-12-2 DMF

RX(5) RCT R 1066-54-2, S **132131-20-5**
RGT T 110-89-4 Piperidine
PRO N 425623-43-4
CAT 3375-31-3 Pd(OAc)2, 7681-65-4 CuI, 6163-58-2
Tri-o-tolylphosphine
SOL 68-12-2 DMF

RX(4) RCT N 425623-43-4
RGT P 429-41-4 Bu4N.F
PRO O 425623-42-3
SOL 109-99-9 THF

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RX(6)      RCT  O 425623-42-3, J 425623-41-2
           RGT  L 121-44-8 Et3N
           PRO  X 425623-44-5
           CAT  14221-01-3 Pd(PPh3)4
           SOL  68-12-2 DMF

RX(7)      RCT  X 425623-44-5
           RGT  Z 1333-74-0 H2
           PRO  A 425623-45-6
           CAT  7440-05-3 Pd
           SOL  75-09-2 CH2Cl2, 67-56-1 MeOH

RX(1)      RCT  A 425623-45-6
           RGT  C 17194-00-2 Ba(OH)2
           PRO  B 425623-39-8
           SOL  67-56-1 MeOH, 7732-18-5 Water
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ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:.
STN INTERNATIONAL LOGOFF AT 16:37:16 ON 25 JUN 2004
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10/627,483 Thomas McKenzie

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1611txm

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	May 10	PROUSDDR now available on STN
NEWS 4	May 19	PROUSDDR: One FREE connect hour, per account, in both May and June 2004
NEWS 5	May 12	EXTEND option available in structure searching
NEWS 6	May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS 7	May 17	FRFULL now available on STN
NEWS 8	May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
NEWS 9	May 27	CAplus super roles and document types searchable in REGISTRY
NEWS 10	May 27	Explore APOLLIT with free connect time in June 2004
NEWS 11	Jun 22	STN Patent Forums to be held July 19-22, 2004

NEWS EXPRESS	MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:30:27 ON 25 JUN 2004

=> file reg
FILE 'REGISTRY' ENTERED AT 17:30:42 ON 25 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 JUN 2004 HIGHEST RN 698838-50-5
DICTIONARY FILE UPDATES: 24 JUN 2004 HIGHEST RN 698838-50-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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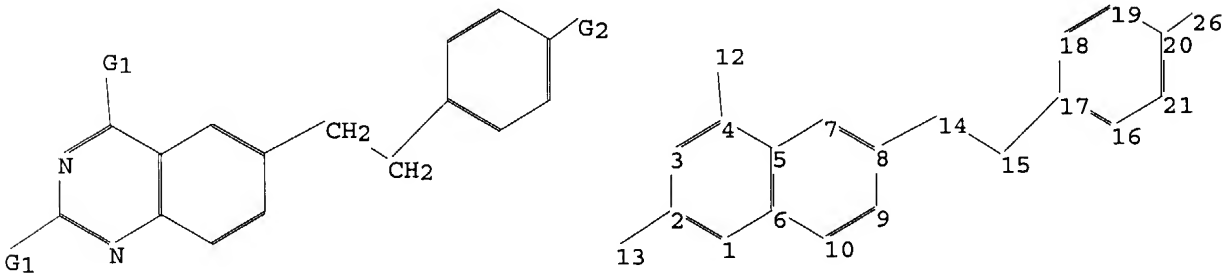

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ring nodes :
1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21
chain bonds :
2-13 4-12 8-14 14-15 15-17 20-26 22-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20 20-21
exact/norm bonds :
2-13 4-12 20-26 22-23
exact bonds :
8-14 14-15 15-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20 20-21

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G1:C,O,N

G2:OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:CLASS 23:CLASS 26:CLASS
fragments assigned product role:
containing 22
fragments assigned reactant/reagent role:
containing 1

L1 STRUCTURE UPLOADED

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SAMPLE SCREEN SEARCH COMPLETED - 10 TO ITERATE

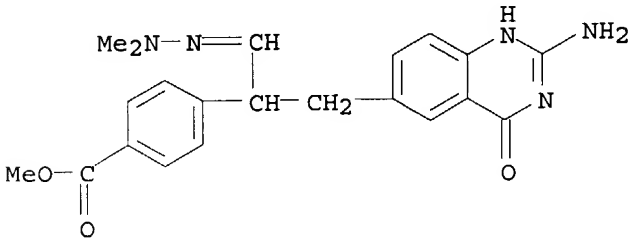
100.0% PROCESSED 10 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 11 TO 389
PROJECTED ANSWERS: 7 TO 298

L2 7 SEA SSS SAM L1

=> d scan

L2 7 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Benzoic acid, 4-[2-(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)-1-[(dimethylhydrazono)methyl]ethyl]-, methyl ester (9CI)
MF C21 H23 N5 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 7 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN L-Glutamic acid, N-[4-[2-(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)-1-bromo-1-(bromomethyl)ethyl]benzoyl]-, bis(1,1-dimethylethyl) ester (9CI)

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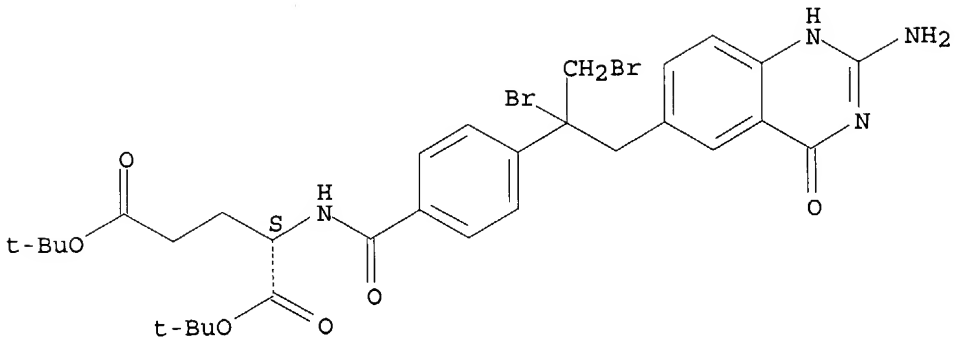
MF C31 H38 Br2 N4 O6

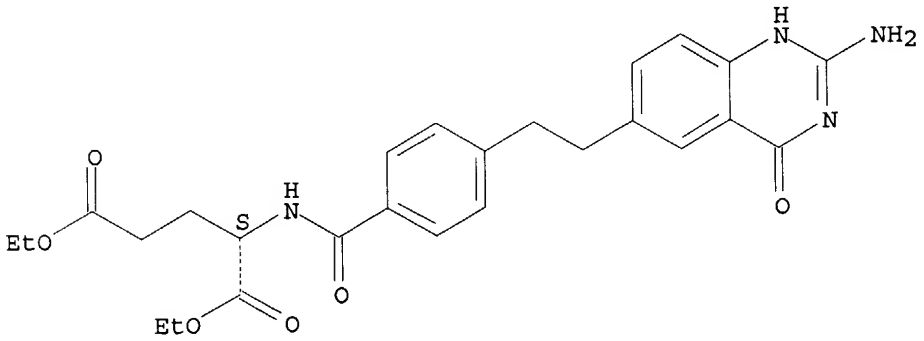
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 7 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN L-Glutamic acid, N-[4-[2-(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)ethyl]benzoyl]-, diethyl ester (9CI)
MF C26 H30 N4 O6

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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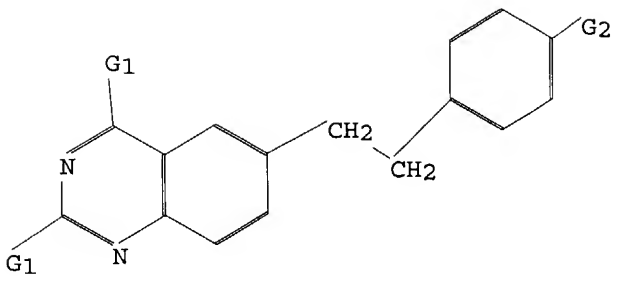

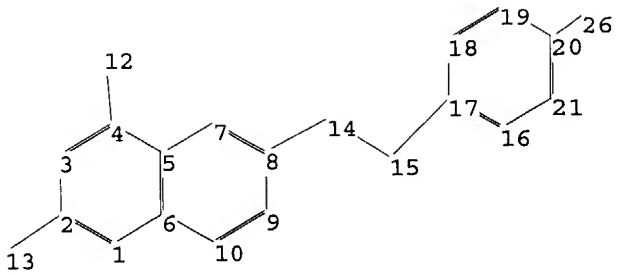

chain nodes :
12 13 14 15 22 23 26
ring nodes :
1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21
chain bonds :
2-13 4-12 8-14 14-15 15-17 20-26 22-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21
exact/norm bonds :
2-13 4-12 20-26 22-23
exact bonds :
8-14 14-15 15-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21

G1:C,O,N

G2:OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:CLASS 23:CLASS 26:CLASS
fragments assigned product role:
containing 22
fragments assigned reactant/reagent role:
containing 1

L3 STRUCTURE UPLOADED

```
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SAMPLE SEARCH INITIATED 17:32:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     10 TO ITERATE

100.0% PROCESSED      10 ITERATIONS                                  2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           11 TO      389
PROJECTED ANSWERS:               2 TO      124

L4             2 SEA SSS SAM L3

=> d scan

L4   2 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   Benzoic acid, 4-[2-(2,4-diamino-6-quinazolinyl)ethyl]- (9CI)
MF   C17 H16 N4 O2
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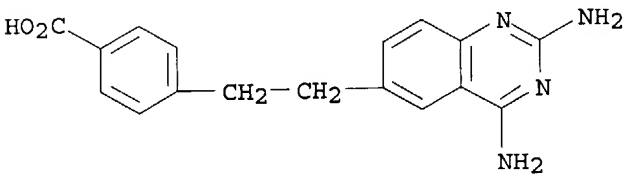


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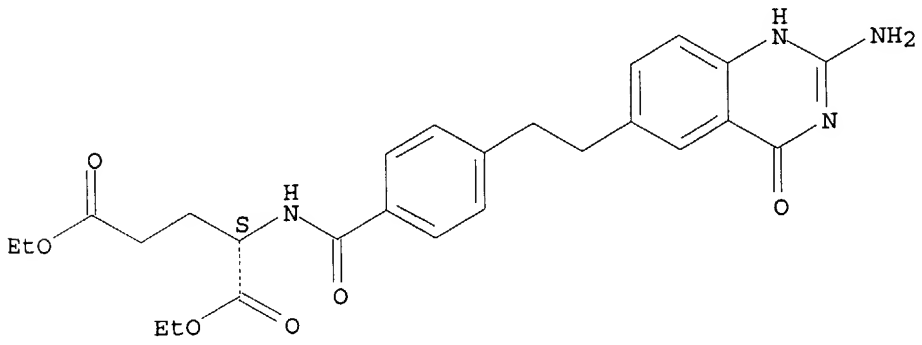
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4   2 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   L-Glutamic acid, N-[4-[2-(2-amino-1,4-dihydro-4-oxo-6-
     quinazolinyl)ethyl]benzoyl]-, diethyl ester (9CI)
MF   C26 H30 N4 O6

Absolute stereochemistry.
```

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
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ALL ANSWERS HAVE BEEN SCANNED

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FULL SEARCH INITIATED 17:32:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     102 TO ITERATE

100.0% PROCESSED     102 ITERATIONS                                  15 ANSWERS
SEARCH TIME: 00.00.01

L5            15 SEA SSS FUL L3

=> file caplus
FILE 'CAPLUS' ENTERED AT 17:33:11 ON 25 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 25 Jun 2004  VOL 141 ISS 1
FILE LAST UPDATED: 24 Jun 2004  (20040624/ED)
```

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l5/p
L6            8 L5/P

=> d 1-8 cbib pi abs hitstr

L6   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2004 ACS on STN
2004:392361   Document No. 140:407108  Process for synthesizing antifolates.
     Xiao, Zejun; Kochat, Harry (USA).  U.S. Pat. Appl. Publ. US 2004092739 A1
     20040513, 7 pp.  (English).  CODEN: USXXCO.  APPLICATION: US 2003-627485
     20030725.  PRIORITY: US 2002-PV425826 20021113.
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ---------------   ----  --------      ---------------  --------
PI   US 2004092739      A1   20040513      US 2003-627485   20030725
     WO 2004045500      A2   20040603      WO 2003-US33237  20031022
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG,
             KZ, MD, RU, TJ
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
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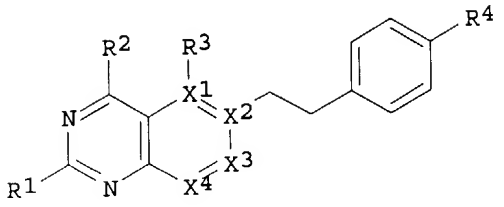
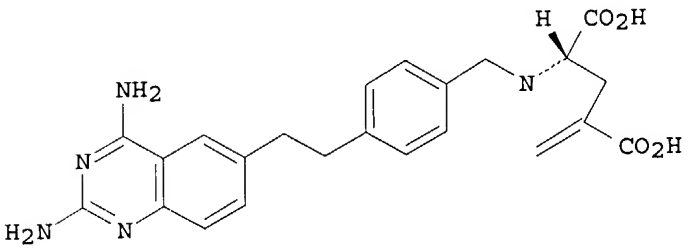
NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

GI



I



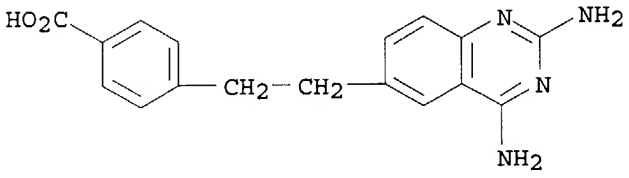
II

AB This invention relates to a process for synthesizing certain folic acid analogs [I; herein R1, R2 = amino or N-alkyl substituted amino, HO, alkoxy, keto, lower alkyl, or a nitrogen or oxygen protecting group; R3 = H, HO, alkoxy, CF3, alkoxy, halo, SH, or alkylthio; R4 = HO, alkoxy, CO-X; wherein X = HO, alkoxy, or an amino acid residue; X1-X4 = carbon or nitrogen], in particular γ-methylene glutamate 5,8,10-trideazaaminopterin (TRIDAM), (II) which are useful in treating cancer, inflammatory diseases, or autoimmune diseases, and are commonly referred to as antifolates (no data). The process employs improved steps for annulation, derivatization and addition reactions to produce the described antifolates from commonly available starting materials. Thus, a mixture of 2-amino-5-methylbenzonitrile and cyanoguanidine in 1 N aqueous HCl solution was heated at reflux for 1.5 h to give, after workup and treatment with aqueous ammonium hydroxide, 2,4-diamino-6-methylquinazoline which was amidated with benzoyl chloride in the presence of Et3N in 1,4-dioxane under heating at reflux for 1 h to give 2,4-dibenzamido-6-methylquinazoline (III). III was brominated by 1,3-dibromo-5,5-dimethylimidazolidine-2,4-dione in the presence of benzoyl peroxide in CCl4 under irradiation with a high intensity lamp (600 W, 120 V) for 1 h to give 2,4-dibenzamido-6-bromomethylquinazoline which was reacted with triphenylphosphine in THF under relaxing for 2 h and underwent Wittig reaction with Me 4-formylbenzoate in the presence of potassium tert-butoxide in THF at 25° for 24 h to give 2,4-Dibenzamido-6-[2-(p-methoxycarbonylphenyl)ethenyl]quinazoline (IV). IV was hydrogenated over 10% Pd-C in DMF at a hydrogen pressure of 20 psi for 20 h to give 2,4-Dibenzamido-6-[p-(methoxycarbonyl)phenethyl]quinazoline which was hydrolyzed in a mixture of 1 N aqueous KOH solution and MeCN under heating at reflux for 42 h and neutralized with AcOH to give 4-amino-4-deoxy-5,8,10-trideazapteroic acid (V). V was condensed with di-Et 4-methylene-L-glutamate hydrochloride in DMF at 25° for 30 min using 1-hydroxybenzotriazole and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide

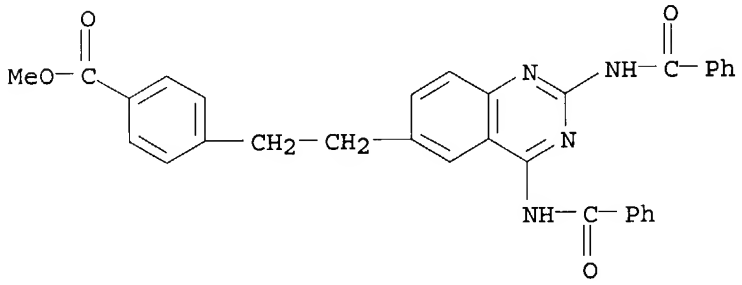
hydrochloride as condensing agents to give di-Et 4-methylene-N-[4-[2-(2,4-diaminoquinazolin-6-yl)ethyl]benzoyl]glutamate, i.e. TRIDAM di-Et ester, which was saponified in a mixture of 1 N aqueous NaOH solution and MeCN at 25° for 16 h and neutralized with AcOH to give TRIDAM II.

IT **227016-65-1P**, 4-Amino-4-deoxy-5,8,10-trideazapteroic acid
688056-38-4P, 2,4-Dibenzamido-6-[p-(methoxycarbonyl)phenethyl]quinazoline **688056-39-5P**, Diethyl 4-methylene-N-[4-[2-(2,4-diaminoquinazolin-6-yl)ethyl]benzoyl]-L-glutamate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for synthesizing antifolates in treating cancer, inflammatory diseases, autoimmune diseases)

RN 227016-65-1 CAPLUS
CN Benzoic acid, 4-[2-(2,4-diamino-6-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)

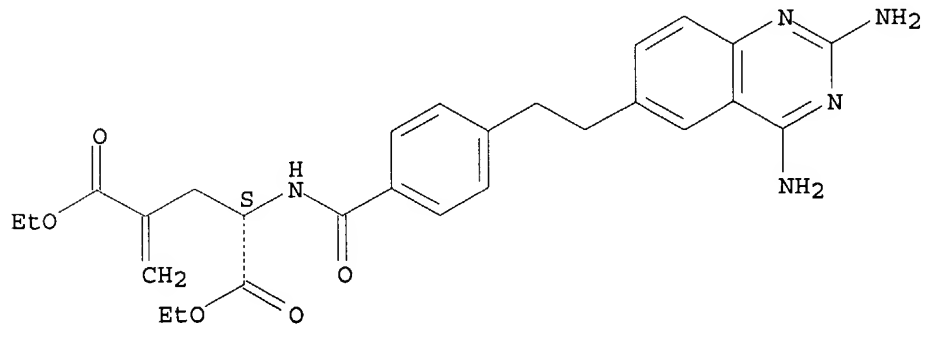


RN 688056-38-4 CAPLUS
CN Benzoic acid, 4-[2-[2,4-bis(benzoylamino)-6-quinazolinyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)



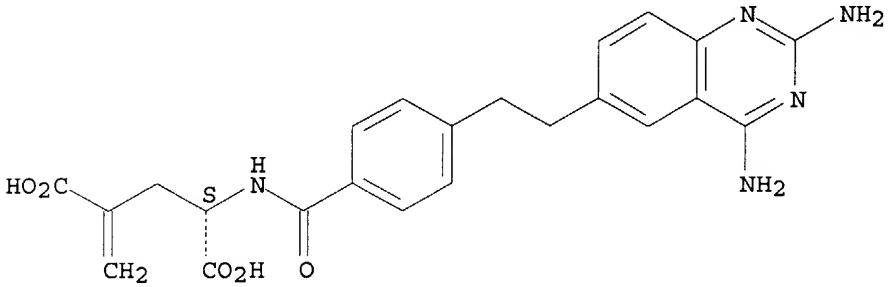
RN 688056-39-5 CAPLUS
CN L-Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]-4-methylene-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

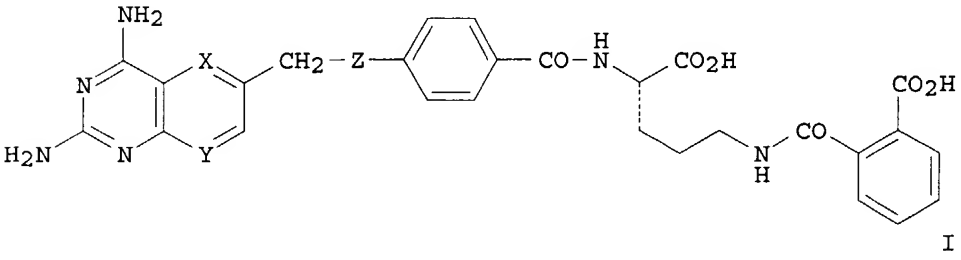


IT **227016-66-2P**, 4-Methylene-N-[4-[2-(2,4-diaminoquinazolin-6-yl)ethyl]benzoyl]-L-glutamic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(process for synthesizing antifolates in treating cancer, inflammatory diseases, autoimmune diseases)
RN 227016-66-2 CAPLUS
CN L-Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]-4-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
2002:197432 Document No. 136:386360 Synthesis and In Vitro Antitumor Activity of New Deaza Analogues of the Nonpolyglutamatable Antifolate Nα-(4-Amino-4-deoxypteroyl)-Nδ-hemiphthaloyl-L-ornithine (PT523). Vaidya, Chitra M.; Wright, Joel E.; Rosowsky, Andre (Dana-Farber Cancer Institute and the Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA). Journal of Medicinal Chemistry, 45(8), 1690-1696 (English) 2002. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 136:386360. Publisher: American Chemical Society.
GI



I

AB Details are disclosed for the synthesis of Nα-[4-[2-(2,4-diaminoquinazolin-6-yl)ethyl]benzoyl]-Nδ-hemiphthaloyl-L-ornithine (2), I (X = Y = CH, Z = CH2), and Nα-[4-[5-(2,4-diaminoteridin-6-yl)pent-1-yn-4-yl]benzoyl]-Nδ-hemiphthaloyl-L-ornithine (6), I [X = Y = N, Z = CH(CH2C.tplbond.CH)], as analogs of Nα-(4-amino-4-deoxypteroyl)-Nδ-hemiphthaloyl-L-ornithine (PT523, 1), I (X = Y = N, Z = NH), a nonpolyglutamatable antifolate currently in advanced preclin. development. In a 72 h growth inhibition assay against cultures of

CCRF-CEM human leukemic lymphoblasts, the IC50 of 2 and 6 was 0.69 ± 0.044 nM and 1.3 ± 0.35 nM, resp., as compared with previously reported values 4.4 ± 0.10 nM for aminopterin (AMT) and 1.5 ± 0.39 nM for PT523. In a spectrophotometric assay of dihydrofolate reductase (DHFR) inhibition using dihydrofolate and NADPH as the cosubstrates, the previously unreported compds. 2 and the mixed 10R and 10S diastereomers of 6 had Ki values of 0.21 ± 0.05 pM and 0.60 ± 0.02 pM, resp., as compared with previously reported values of 3.70 ± 0.35 pM for AMT and 0.33 ± 0.04 pM for PT523. Thus, while they were comparable to PT523 and several of its previously studied analogs in their ability to bind to DHFR and inhibit the growth of CCRF-CEM cells, 2 and the mixed diastereomers of 6 were several times more active than AMT despite the fact that they cannot form γ-polyglutamylated metabolites of the type formed in cells from AMT and other classical antifolates with a glutamate side chain.

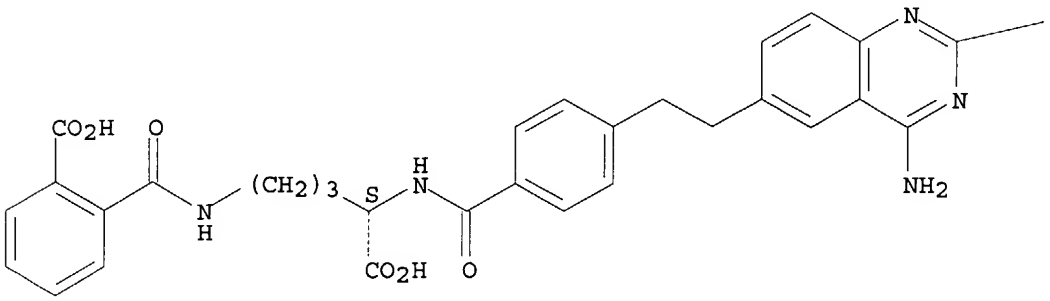
IT **425623-39-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and in vitro antitumor activity of deaza analogs of the nonpolyglutamatable antifolate PT-523)

RN 425623-39-8 CAPLUS

CN Benzoic acid, 2-[[[(4S)-4-carboxy-4-[[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]amino]butyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

—NH2

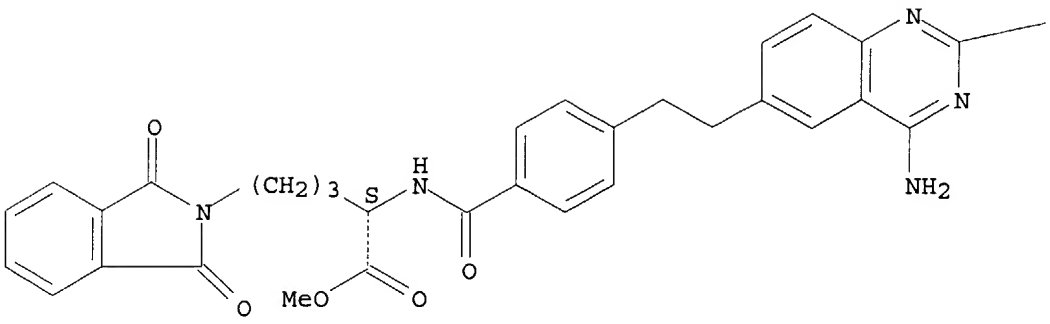
IT **425623-45-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and in vitro antitumor activity of deaza analogs of the nonpolyglutamatable antifolate PT-523)

RN 425623-45-6 CAPLUS

CN 2H-Isoindole-2-pentanoic acid, α-[[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

—NH_2

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
1999:384008 Document No. 131:32168 Synthesis of 4-amino-4-deoxy-5,8,10-trideazapteroyl-4'-methyleneglutamic acid as metabolically inert antiinflammatory and antitumor antifolates. Nair, Madhavan G. (USA). U.S. US 5912251 A 19990615, 9 pp. (English). CODEN: USXXAM.
APPLICATION: US 1998-8613 19980117.

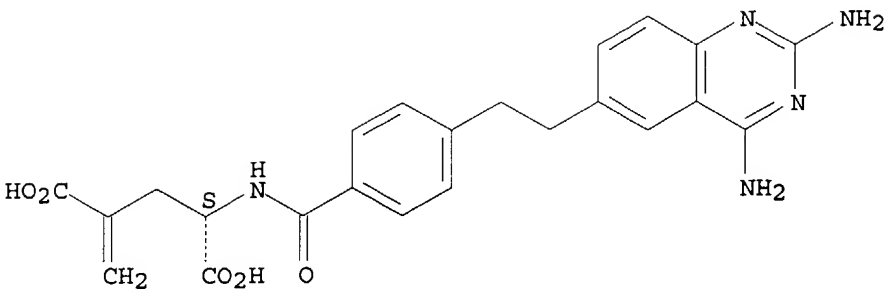
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5912251	A	19990615	US 1998-8613	19980117
	WO 9936409	A1	19990722	WO 1999-US948	19990113
	W: JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 1062209	A1	20001227	EP 1999-903128	19990113
	R: CH, DE, GB, LI				
	JP 2002509139	T2	20020326	JP 2000-540125	19990113

AB 4-Amino-4-deoxy-5,8,10-trideazapteroyl-4'-methyleneglutamic acid (1) and related compds. were prepared as antiinflammatory and antitumor agents. The synthesis of 1 involved coupling of 5-methyl-2-nitrobenzonitrile with Me 4-formylbenzoate, dithionite reduction, guanidine cyclization, saponification, hydrogenation, and coupling with di-Et 4-methyleneglutamate. Compound 1 was 1,000 to 10,000 times more active than methotrexate in causing total growth inhibition of a number of human tumor cells in culture.

IT **227016-66-2P 227016-75-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of aminodeoxytrideazapteroylmethyleneglutamic acid as metabolically inert antiinflammatory and antitumor antifolates)

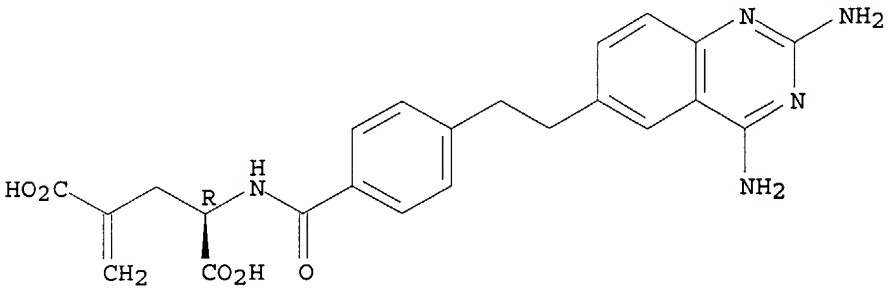
RN 227016-66-2 CAPLUS
CN L-Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]-4-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

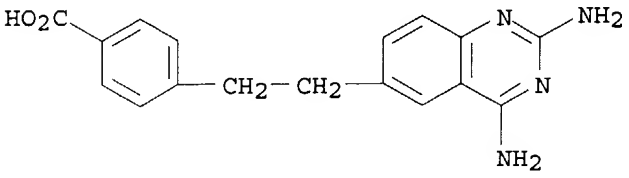


RN 227016-75-3 CAPLUS
CN D-Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]-4-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



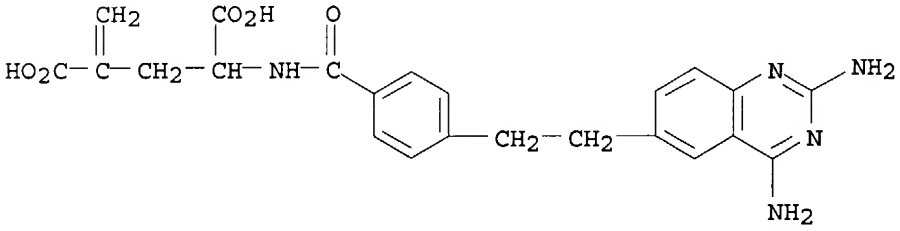
IT **227016-65-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of aminodeoxytrideazapteroylmethyleneglutamic acid as metabolically inert antiinflammatory and antitumor antifolates)
RN 227016-65-1 CAPLUS
CN Benzoic acid, 4-[2-(2,4-diamino-6-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



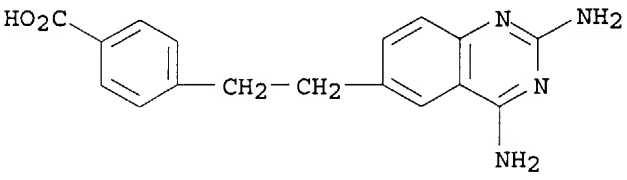
L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
1999:368950 Document No. 131:166959 Metabolism blocked classical folate analog inhibitors of dihydrofolate reductase-1: synthesis and biological evaluation of mobiletrex. Nair, M. Gopal; Fayard, Melanie L.; Lariccia, Joanna M.; Amato, Alaina E.; McGuire, John J.; Galivan, John H.; Kisliuk, Roy L. (Department of Biochemistry and Molecular Biology, University of South Alabama, Mobile, AL, 36688, USA). Medicinal Chemistry Research, 9(3), 176-185 (English) 1999. CODEN: MCREEB. ISSN: 1054-2523. OTHER SOURCES: CASREACT 131:166959. Publisher: Birkhaeuser Boston.
AB A classical folate analog inhibitor of dihydrofolate reductase is

described. This compound, 4'-methylene-5,8,10-trideazaaminopterin [Mobiletrex; M-Trex], is resistant to both polyglutamylation and aldehyde oxidase mediated 7-hydroxylation. Mobiletrex exhibited excellent inhibition of human dihydrofolate reductase and inhibited growth of a number of human tumor cells in culture. Unlike methotrexate, mobiletrex was not a substrate of either folylpolyglutamate synthetase or rabbit liver aldehyde oxidase. Mobiletrex caused total growth inhibition (TGI) of a number of human tumor cells at therapeutically relevant concns. (.apprx. 1+10-6 M) which are potencies strikingly higher than those of methotrexate.

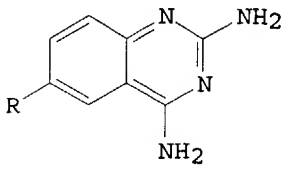
IT **238074-89-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of folate analog inhibitor of dihydrofolate reductase-1)
RN 238074-89-0 CAPLUS
CN Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]-4-methylene- (9CI) (CA INDEX NAME)



IT **227016-65-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of folate analog inhibitor of dihydrofolate reductase-1)
RN 227016-65-1 CAPLUS
CN Benzoic acid, 4-[2-(2,4-diamino-6-quinazolinyl)ethyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
1992:255573 Document No. 116:255573 Antifolate and antibacterial activities of 6-substituted 2,4-diaminoquinazolines. Harris, N. V.; Smith, C.; Bowden, K. (Dagenham Res. Cent., Rhone-Poulenc Rorer Ltd., Dagenham/Essex, UK). European Journal of Medicinal Chemistry, 27(1), 7-18 (English) 1992. CODEN: EJMCA5. ISSN: 0223-5234.
GI



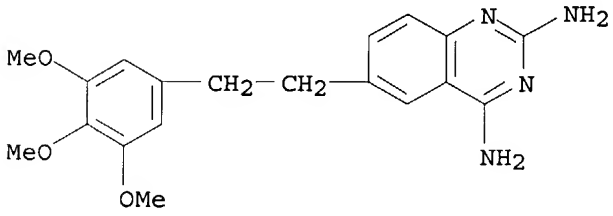
I

AB 6-Substituted 2,4-diaminoquinazolines are good inhibitors of dihydrofolate reductase (DHFR) and effective as growth inhibitors of intact bacterial cells in vitro. Therefore, quinazolines I [R = iodo, NMe2, C.tplbond.C(CH2)4Me, (CH2)6Me, CH2CH2Ph, (Z)-CH:CHPh, etc.] were prepared and tested for DHFR inhibition and antibacterial activity. Thus, iodination of 2-H2NC6H4CN and cyclization with chloroformamidine gave I (R = iodo) in 30% yield. The most potent compds. in the in vitro tests were, however, ineffective against a systemic murine infection. Quant. correlations were obtained between DHFR inhibition and the substituent constant molar refractivity (MR) for 3 of the 4 enzymes studied (Escherichia coli, Streptococcus faecalis, and bovine liver (DHFR); for the fourth enzyme (Staphylococcus aureus DHFR) the best correlation was obtained with a combination of MR and the lipophilic parameter π. From these results it was possible to construct a simple schematic model of the binding site occupied by the 6-substituents; a subsequent mol. modeling study agreed with the features of this model.

IT **141400-19-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, bactericidal, and dihydrofolate inhibitory activity of)

RN 141400-19-3 CAPLUS

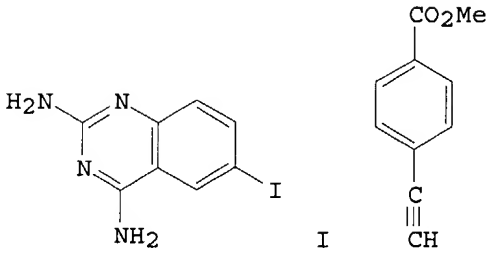
CN 2,4-Quinazolinediamine, 6-[2-(3,4,5-trimethoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN

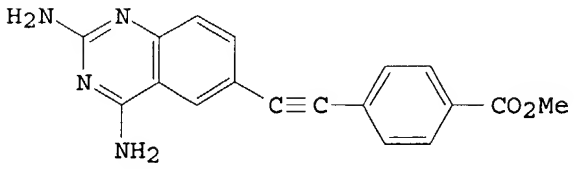
1991:102721 Document No. 114:102721 A simple synthesis of 5,8,10-trideazaminopterin analogs. Harris, Neil V.; Smith, Christopher; Bowden, Keith (Dagenham Res. Cent., Rhone-Poulenc (UK) Ltd., Dagenham/Essex, UK). Synlett (10), 577-8 (English) 1990. CODEN: SYNLES. ISSN: 0936-5214. OTHER SOURCES: CASREACT 114:102721.

GI

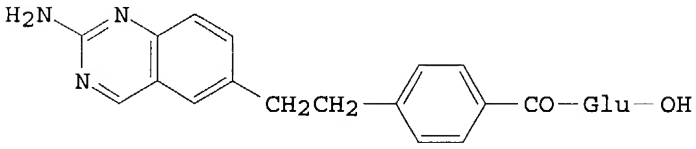


I

II



III



IV

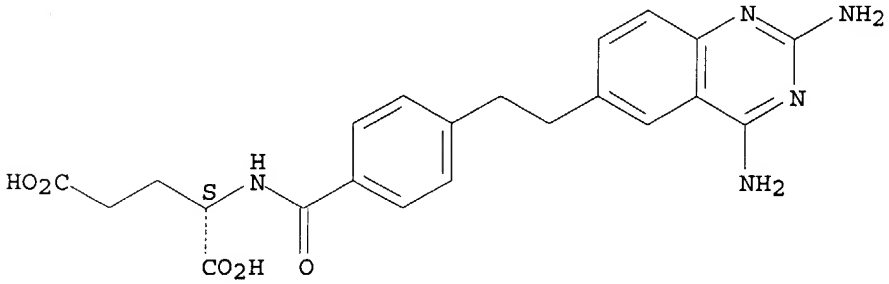
AB The Heck reaction between 6-iodoquinozoline I and benzoate II gave 95% quinazoline III. II was converted into 5,8,10-trideazaaminopterin IV, the quinazoline analog of 10-deazaminopterin.

IT **70583-37-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dihydrofolate reductase-inhibiting activity of)

RN 70583-37-8 CAPLUS

CN L-Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

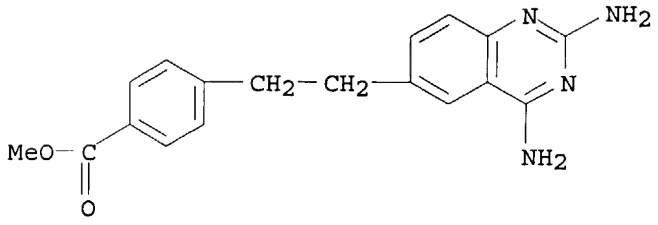
Absolute stereochemistry.



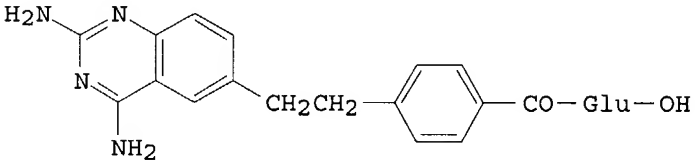
IT **132131-25-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for trideazaminopterine)

RN 132131-25-0 CAPLUS

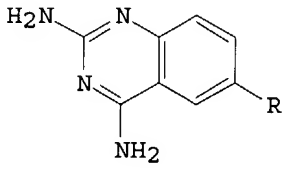
CN Benzoic acid, 4-[2-(2,4-diamino-6-quinazolinyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
1979:421042 Document No. 91:21042 Folic acid analogs. III. N-(2-[2-(2,4-Diamino-6-quinazolinyl)ethyl]benzoyl)-L-glutamic acid. Yan, S. J.; Weinstock, Louis T.; Cheng, C. C. (Midwest Res. Inst., Kansas City, MO, 64110, USA). Journal of Heterocyclic Chemistry, 16(3), 541-4 (English) 1979. CODEN: JHTCAD. ISSN: 0022-152X.
GI



I



II

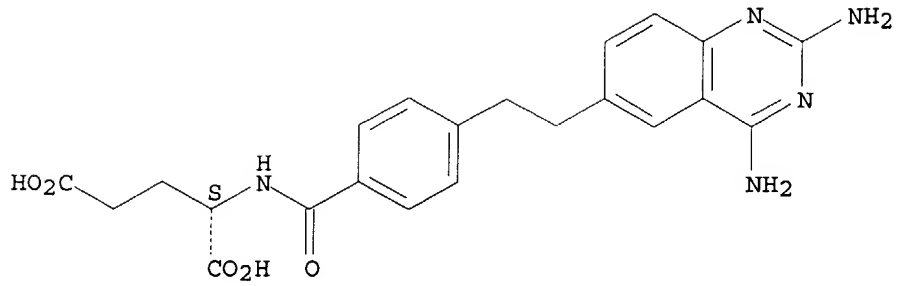
AB A trideaza analog (I) of aminopterin was prepared by Wittig condensation of diaminoquinazolinecarboxaldehyde II (R = CHO) and 4-(Ph3P+CH2)C6H4CO-Glu(OEt)-OEt.Br- (III) and subsequent hydrogenation and hydrolysis. I inhibited leukemia L1210 in mice at 0.08 mg/kg. II (R = CHO) was prepared from 2,5-(H2N)(O2N)C6H3CN by cyclocondensation with guanidine to give II (R = NO2) (IV). Reduction of IV gave II (R = NH2), which was diazotized and treated with CuCN to give II (R = CN). Reduction of the latter in aqueous HOAc containing PhNHNH2 gave II (R = CH:NNHPh) which was hydrolyzed to give II (R = CHO). III was prepared by acylation of H-Glu(OEt)-OEt with 4-BrCH2C6H4COBr and subsequent treatment with Ph3P.

IT **70583-37-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antileukemia activity of)

RN 70583-37-8 CAPLUS

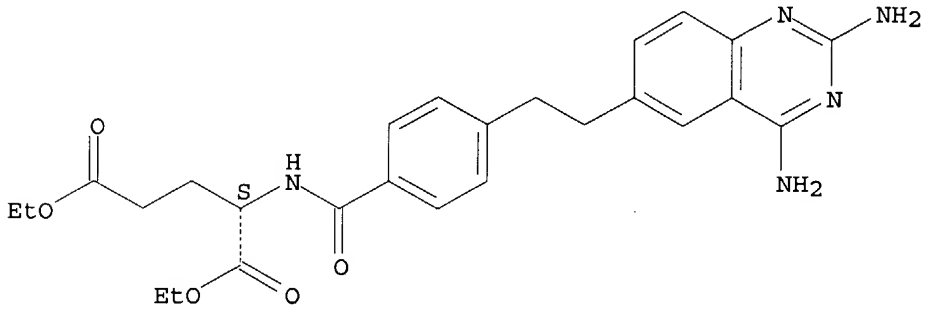
CN L-Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

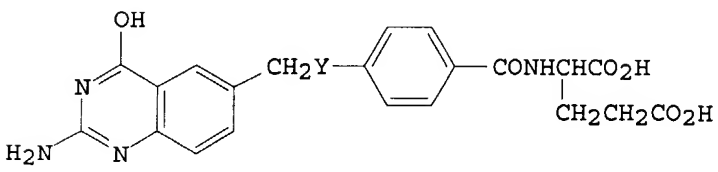


IT **70583-36-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 70583-36-7 CAPLUS
CN L-Glutamic acid, N-[4-[2-(2,4-diamino-6-quinazolinyl)ethyl]benzoyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
1977:561582 Document No. 87:161582 Synthesis of quinazoline analogs of folic acid modified at position 10. Oatis, John E., Jr.; Hynes, John B. (Dep. Pharm. Chem., Med. Univ. South Carolina, Charleston, SC, USA). Journal of Medicinal Chemistry, 20(11), 1393-6 (English) 1977. CODEN: JMCMAR. ISSN: 0022-2623.
GI



I, Y=S
II, Y=O
III, Y=CH_2

AB Three title analogs, 5,8-deaza-10-thiafolic acid (I) [64088-74-0], 5,8-deaza-10-oxafolic acid (II) [64088-76-2], and 5,8,10-deazafolic acid (III) [64088-73-9] were prepared and found to have marginal activity against L1210 leukemia in mice at 150 mg/kg, i.p., with no evidence of acute

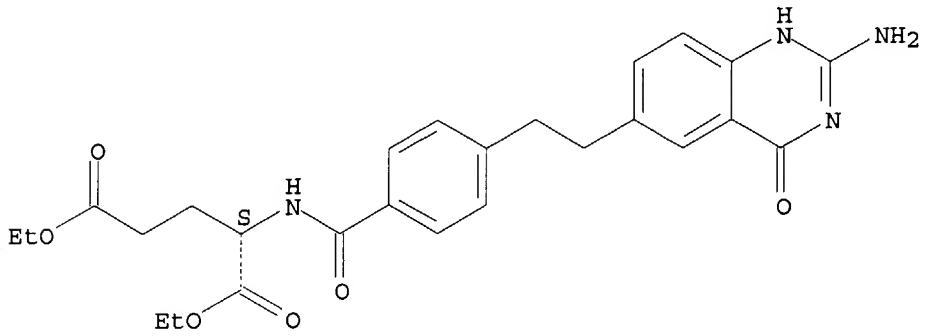
toxicity.

IT **64088-73-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and leukemia inhibiting activity of)

RN 64088-73-9 CAPLUS

CN L-Glutamic acid, N-[4-[2-(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)ethyl]benzoyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and saponification of

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